REPORT:

2nd TwiNSol-CECs Training

"*High-resolution mass spectrometry application in revealing the CECs presence in water*"

The second TwiNSol-CECs Training was organized within TwiNSol-CECs project (101059867) as a five-day event on November 21-25, 2022 at the partner institution, the Spanish National Research Council, Institute of Environmental Assessment and Water Research (CSIC), Barcelona, Spain. It was attended by two representatives of TFNS team members: Dr. Jelena Živančev and Dr. Igor Antić, who both have significant knowledge in application of various MS detection-based analytical techniques.

Before the Training, online pre-training session was held to introduce the TFNS members from the UHPLC-MS lab with basics of surface water sampling and preparation for subsequent screening analysis. This online meeting held on Nov 04, 2022, was led by Dr. Marinella Farre, CSIC Project Manager, and it was attended by the whole CSIC team and TFNS members from the UHPLC-MS lab. The procedure for the surface water samples preparation for subsequent CECs screening was explained by CSIC team members (column conditioning, loading of samples, washing, and drying) and it was practiced at TFNS lab before the 2nd TwiNSol-CECs training as a preparatory step for the following advanced training session at CSIC.

Agenda of the 2nd TwiNSol-CECs training is attached and it consists of practical lessons and necessary work within different, consecutive phases of the CECs screening methods for analysis of per- and polyfluoroalkyl substances (PFSA) and pharmaceutically active compounds (PhACs). The presented methods are those previously developed and valorized by CSIC researchers involved in TwiNSol-CECs project. These methods have been used in CSIC labs for determination of CECs occurrence in different samples, with the results published in highly ranked international journals.

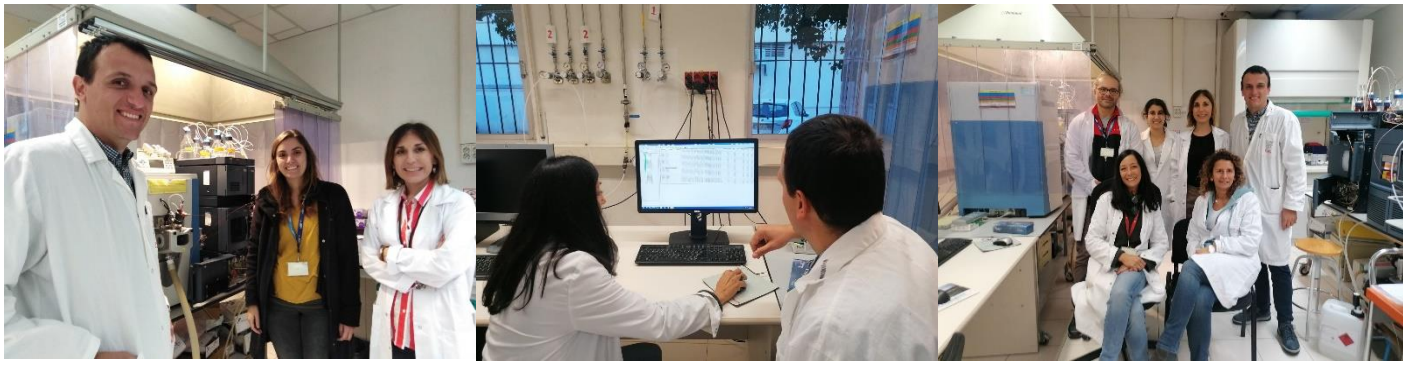
Before starting the demonstration of high-resolution mas spectrometric analysis, Dr. Llorka gave a theoretical introduction about HPLC-HRMS (Q-Exactive) technique, introducing the trainees, Dr. Živančev and Dr. Antić, with HPLC columns, MS ion source, mobile phases, and the whole analytical procedures and conditions for analysis of PFSA. Dr. Llorca, Dr. Živančev, and Dr. Antić jointly prepared the sequence for the targeted and then for the suspect screening analysis of PFSA and set the chromatographic and instrumental parameters to start the analysis.

In the same analytical manner, training continued with targeted and suspect screening analysis of PhACs in water extracts, where the role of moderator was played by Olga Gómez.

Introduction to data processing and analysis by a dedicated software tool such as Compound Discoverer Software was delivered by Dr. Farre, Dr. Pérez and Dr. Montemurro. This was of particular importance for the TFNS team and the TwiNSol-CECs project as purchase of Compound Discoverer Software is underway within the project with attention to be used for processing of raw data obtained by the existing UHPLC-HRMS installed at TFNS.

Practicing water sample preparation at TFNS as a follow-up of the online training with CSIC, which served as a preparatory session for 2nd TwiNSol-CECs training

Training session at CSIC on water sample preparation for subsequent targeted and suspect screening analysis of PFSAs and PhACs



Training session at CSIC on HPLC-HRMS analysis

Training session at CSIC on data processing by Compound Discoverer software

2nd TwiNSol-CECs Training

"High-resolution mass spectrometry application in revealing the CECs presence in water"

organized at Spanish National Research Council, Institute of Environmental Assessment and Water Research (CSIC), Spain,

within the TwiNSol-CECs project (101059867)

21-25 November 2022

PROGRAM

21.11.2022.

09,00-17,00 Extraction of CECs from water samples using homemade cartridges

13,00-14,00 Lunch break

22.11.2022.

09,00-17,00 Extraction of CECs from water samples using commercial single bed cartridges

13,00-14,00 Lunch break

23.11.2022.

09,00-17,00 Target and suspect screening analysis of PFAS in water samples

13,00-14,00 Lunch break

24.11.2022.

09,00-17,00 Target and suspect screening analysis of PhACs in water samples

13,00-14,00 Lunch break

25.11.2022.

09,00-17,00 Introduction to data analysis by Compound Discoverer Software

13,00-14,00 Lunch break

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or EU executive agency. Neither the European Union nor the granting authority can be held responsible for them.